

1,5-Dimethyl-6-phenyl-1,6-dihydro-3-pyridinecarbonitrile  
27531-49-3 | DTXSID30297547

Model Performance

Model

Data

Weighted KNN model

| 5-fold CV (75%) |      | Training (75%) |      | Test (25%) |      |
|-----------------|------|----------------|------|------------|------|
| Q2              | RMSE | R2             | RMSE | R2         | RMSE |
| 0.84            | 0.55 | 0.85           | 0.53 | 0.83       | 0.64 |

Model Results

Predicted value: 11.0

Global applicability domain: Inside

Local applicability domain index: 4.97e-01

Confidence level: 5.16e-01

Nearest Neighbors from the Training Set

|  |   |  |
|--|---|--|
| <div>Image not found</div> <div>Thiram</div> <div>Measured: 3.39</div> <div>Predicted: 3.91</div>        | <div>Image not found</div> <div>Isophorone</div> <div>Measured: 2.00</div> <div>Predicted: 3.19</div>                         | <div>Image not found</div> <div>2-(Thiocyanomethylthio)benzothiazole</div> <div>Measured: 209</div> <div>Predicted: 13.0</div> |
| <div>Image not found</div> <div>Triallylamine</div> <div>Measured: 3.55</div> <div>Predicted: 4.23</div> | <div>Image not found</div> <div>N,N-Dimethyl-1,2-dithiolan-4-amine</div> <div>Measured: 52.5</div> <div>Predicted: 17.5</div> |  |